

# Path Integral Approach to the Non-Relativistic Electron Charge Transfer

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November 2, 2001

## Abstract

A path integral approach has been generalized for the non-relativistic electron charge transfer processes. The charge transfer - the capture of an electron by an ion passing another atom, or more generally the problem of rearrangement collisions is formulated in terms of influence functionals. It has been shown that the electron charge transfer process can be treated either as electron transition problem or as elastic scattering of ion and atom in the some effective potential field. The first-order Born approximation for the electron charge transfer cross section has been reproduced to prove the adequacy of the path integral approach for this problem.

*PACS* number(s): 03.65.Db, 03.65.Nk, 34.70.+e

## 1 Introduction

The path integral approach to quantum mechanics proposed by Feynman [1] today is the efficient tool of theoretical physics. The path integrals play

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an important role in quantum field theory [2], [3], [4], [5] statistical physics and theory of critical phenomena [6], [7], [8] quantum optics [9], theory of stochastic processes [10], [11].

However, up to now path integrals have not been applied to atomic physics problem - electron charge transfer processes. We generalize the path integral approach to the problem of the rearrangement collisions and, in particular, to the capture of an electron by an ion passing another atom. It is so-called the electron charge transfer process. The charge transfer process is an important atomic physics process. Besides the intrinsic interest in the charge transfer as a fundamental physical process, a knowledge of its mechanisms is a prerequisite for an understanding of radiation detectors, radiation damage in matter, injection into thermonuclear fusion systems, astrophysical processes, gas discharges, mass spectrometry and numerous other practical devices.

The theory of the charge transfer reactions based on the traditional quantum-mechanical approaches can be found in the set of monographs (see, for example, [12], [13]). The recent experimental data and references can be found in [14], [15].

In the framework of the path integral approach we have reformulated the problem of calculation of charge transfer cross section. We have developed two new alternative quantum mechanical influence functionals in the problem of the electron charge transfer. We treat the electron charge transfer process either as an electron transition problem or as an reciprocal elastic scattering of ion and atom in the some effective potential field.

The paper is organized as follows.

In Sec.2 we develop the path integral approach to elastic scattering problem. As an application of the developed approach we have reproduced the well known equation for differential cross section in the first-order Born approximation.

In Sec.3 we have generalized the path integral approach to atomic physics rearrangement collisions problem. The cross section for the electron charge transfer process is expressed in the terms of the path integral.

## 2 Elastic scattering cross section. Path integral approach

As was shown by R. Feynman [1], it is possible to describe the quantum mechanical system in terms of the transition amplitude  $K(\mathbf{r}_b, t_b, \mathbf{r}_a, t_a)$ ,

$$K(\mathbf{r}_b, t_b, \mathbf{r}_a, t_a) = \int D\mathbf{r}(\tau) \exp \left\{ \frac{i}{\hbar} S(\mathbf{r}(\tau)) \right\}, \quad (1)$$

where  $a \equiv (\mathbf{r}_a, t_a)$  is the "start point" and  $b \equiv (\mathbf{r}_b, t_b)$  is the "end point" of the quantum-mechanical evolution,  $D\mathbf{r}(\tau)$  means integration over all possible trajectories  $\mathbf{r}(\tau)$ ,  $S(\mathbf{r}(\tau))$  is the classical action of the mechanical system as a functional of its trajectory  $\mathbf{r}(\tau)$ , and  $\hbar$  is the Planck's constant.

In order to clarify the meaning of the above expressions we observe the particle of the mass  $m$  moving in the potential field  $V(\mathbf{r})$ . The classical action for this mechanical system is given by

$$S(\mathbf{r}(\tau)) = \int_{t_a}^{t_b} d\tau \left( \frac{m \dot{\mathbf{r}}^2(\tau)}{2} - V(\mathbf{r}(\tau)) \right). \quad (2)$$

We divide the time interval  $t_b - t_a$  into  $N$  steps of width  $\varepsilon = (t_b - t_a)/N$ . Then the functional  $S(\mathbf{r}(\tau))$  can be represented by the function  $S(\mathbf{r}_a, \mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_{N-1}, \mathbf{r}_b)$ , where  $\mathbf{r}_i = \mathbf{r}(t_i)$  are the points which coincide with the trajectory  $\mathbf{r}(t)$  at the moments  $t_i$  ( $i = 0, 1, \dots, N-1$ ,  $t_0 = t_a$ ,  $t_N = t_b$ ). Hence, the path integral given by Eq.(1) can be written as follows

$$K(\mathbf{r}_b, t_b, \mathbf{r}_a, t_a) = \lim_{N \rightarrow \infty} \left( \frac{m}{2\pi i \varepsilon \hbar} \right)^{3N/2} \int \dots \int d\mathbf{r}_1 \dots d\mathbf{r}_{N-1} \times \\ \times \exp \left\{ \frac{im}{2\hbar\varepsilon} \sum_{j=1}^N (\mathbf{r}_j - \mathbf{r}_{j-1})^2 - \frac{i}{\hbar} \varepsilon \sum_{j=0}^N V(\mathbf{r}_j) \right\}, \quad (3)$$

where  $\mathbf{r}_0 \equiv \mathbf{r}_a$ ,  $\mathbf{r}_N \equiv \mathbf{r}_b$ .

The Eq.(3) presents the transition quantum mechanical amplitude

$K(\mathbf{r}_b, t_b, \mathbf{r}_a, t_a)$  from the point  $a$  to the point  $b$ .

Let us show how to apply the path integral approach to some known atomic physics problems. Consider the scattering of a non relativistic electron on the central potential  $V(|\mathbf{r}|)$ . Being outside of the interaction region (we

assume that the potential is different from zero only in some local area) the electron moves as a free particle. Hence the wave function of the incident electron is just a plane wave

$$\psi(\mathbf{r}_a, t_a) = \exp\left\{\frac{i\mathbf{p}_a\mathbf{r}_a}{\hbar} - \frac{iE_at_a}{\hbar}\right\}, \quad (4)$$

where  $\mathbf{p}_a$  is the electron momentum and  $E_a = p_a^2/2m$  is the electron energy. The normalization of the wave function  $\psi(\mathbf{r}_a, t_a)$  is chosen in such way that the incident flux  $\mathbf{j}_a$  will be equal to the electron velocity

$$\mathbf{j}_a = \frac{\hbar}{2mi}(\psi^* \frac{\partial}{\partial \mathbf{r}_a} \psi - \psi \frac{\partial}{\partial \mathbf{r}_a} \psi^*) = \frac{\mathbf{p}_a}{m}. \quad (5)$$

Then the knowledge of the transition amplitude and "fixing" of initial state of physical system give the general solution for the evolution of a quantum mechanical system in the potential  $V(\mathbf{r})$

$$\psi(\mathbf{r}_b, t_b) = \int d\mathbf{r}_a K(\mathbf{r}_b, t_b, \mathbf{r}_a, t_a) \psi(\mathbf{r}_a, t_a). \quad (6)$$

Since we are only interested in the elastic scattering cross section we should exclude un-scattered component of the total flux. This component is due to "unperturbed" (or free) evolution of the incident particles. Hence, we have the following expression for the wave function  $\psi_{scat}(\mathbf{r}_b, t_b)$  of the final states of our interest

$$\psi_{scat}(\mathbf{r}_b, t_b) = \int d\mathbf{r}_a \left( K(\mathbf{r}_b, t_b, \mathbf{r}_a, t_a) - K^{(0)}(\mathbf{r}_b, t_b, \mathbf{r}_a, t_a) \right) \psi(\mathbf{r}_a, t_a), \quad (7)$$

where the free (unperturbed) particle transition amplitude  $K^{(0)}(\mathbf{r}_b, t_b, \mathbf{r}_a, t_a)$  is given by

$$\begin{aligned} & K^{(0)}(\mathbf{r}_b, t_b, \mathbf{r}_a, t_a) \\ &= \lim_{N \rightarrow \infty} \left( \frac{m}{2\pi i \varepsilon \hbar} \right)^{3N/2} \int \dots \int d\mathbf{r}_1 \dots d\mathbf{r}_{N-1} \exp \left\{ \frac{im}{2\hbar \varepsilon} \sum_{j=1}^N (\mathbf{r}_j - \mathbf{r}_{j-1})^2 \right\} \end{aligned} \quad (8)$$

$$= \left( \frac{m}{2\pi i \hbar (t_b - t_a)} \right)^{3/2} \exp \left\{ \frac{im}{2\hbar} \frac{|\mathbf{r}_b - \mathbf{r}_a|^2}{t_b - t_a} \right\}.$$

Taking into account the definitions given by Eqs.(6) - (8) the wave function  $\psi_{scat}(\mathbf{r}_b, t_b)$  can be written as

$$\begin{aligned} \psi_{scat}(\mathbf{r}_b, t_b) = & \int d\mathbf{r}_a \psi(\mathbf{r}_a, t_a) \lim_{N \rightarrow \infty} \left( \frac{m}{2\pi i \varepsilon \hbar} \right)^{3N/2} \times \int \dots \int d\mathbf{r}_1 \dots d\mathbf{r}_{N-1} \times \\ & \times \exp \left\{ \frac{im}{2\hbar \varepsilon} \sum_{j=1}^N (\mathbf{r}_j - \mathbf{r}_{j-1})^2 \right\} \times \left( e^{-\frac{i}{\hbar} \varepsilon \sum_{j=0}^N V(\mathbf{r}_j)} - 1 \right). \end{aligned} \quad (9)$$

Physical characteristic of the scattering process is the differential scattering cross section  $d\sigma(\theta, \varphi)$ . It is defined as the ratio of the number of particles scattered into the solid angle  $d\Omega = \sin\theta d\theta d\varphi$  per unit time to the flux density of the incident particles. There are  $j_b r_b^2 d\Omega$  particles (electrons) that pass through the elementary area  $r_b^2 d\Omega$  per unit time. Here  $j_b$  is the radial component of the particle flux density

$$j_b = \frac{\hbar}{2mi} \left( \psi_{scat}^* \frac{\partial}{\partial r_b} \psi_{scat} - \psi_{scat} \frac{\partial}{\partial r_b} \psi_{scat}^* \right). \quad (10)$$

Hence the differential cross section is defined by the following equation [16]

$$d\sigma = \frac{j_b r_b^2 d\Omega}{|\mathbf{j}_a|}, \quad (11)$$

where  $\mathbf{j}_a$  and  $j_b$  are given by Eq.(5) and Eq.(10) reciprocally.

Thus, Eqs.(9)-(11) are the path integral approach to the non-relativistic quantum mechanical problem of elastic scattering. Let us show that in first-order perturbation theory Eqs.(9)-(11) give the well known result of the quantum mechanical scattering theory (the first-order Born approximation, [16]).

In the first order on the  $V(|\mathbf{r}|)$  Eq.(9) can be written as

$$\psi_{scat}(\mathbf{r}_b, t_b) = -\frac{i}{\hbar} \int d\mathbf{r}_a \psi(\mathbf{r}_a, t_a) \lim_{N \rightarrow \infty} \left( \frac{m}{2\pi i \varepsilon \hbar} \right)^{3N/2} \times$$

$$\int \dots \int d\mathbf{r}_1 \dots d\mathbf{r}_{N-1} \exp \left\{ \frac{im}{2\hbar\varepsilon} \sum_{j=1}^N (\mathbf{r}_j - \mathbf{r}_{j-1})^2 \right\} \times \varepsilon \sum_{j=0}^N V(|\mathbf{r}_j|). \quad (12)$$

If the wave function  $\psi(\mathbf{r}_a, t_a)$  is defined according to Eq.(4) then Eq.(12) is read

$$\psi_{scat}(\mathbf{r}_b, t_b) = -\frac{i}{\hbar} \int d\mathbf{r}_a \int_{t_a}^{t_b} d\tau \int d\mathbf{r} K^{(0)}(\mathbf{r}_b, t_b, \mathbf{r}, \tau) V(|\mathbf{r}|) \times \quad (13)$$

$$K^{(0)}(\mathbf{r}, \tau; \mathbf{r}_a, t_a) \exp \left\{ \frac{i\mathbf{p}_a \mathbf{r}_a}{\hbar} - \frac{iE_a t_a}{\hbar} \right\}.$$

Here  $K^{(0)}(\mathbf{r}_b, t_b, \mathbf{r}_a, t_a)$  is the free particle quantum mechanical transition amplitude given by Eq.(8). It is convenient to present Eq.(8) as the Fourier integral

$$K^{(0)}(\mathbf{r}_b, t_b, \mathbf{r}_a, t_a) = \frac{1}{(2\pi\hbar)^3} \int d\mathbf{p} \exp \left\{ -\frac{i\mathbf{p}_a(\mathbf{r}_b - \mathbf{r}_a)}{\hbar} - \frac{ip_a^2(t_b - t_a)}{2m\hbar} \right\}.$$

Substituting the above equation for  $K^{(0)}$  in Eq.(13) yields

$$\begin{aligned} \psi_{scat}(\mathbf{r}_b, t_b) = & -\frac{i}{\hbar} \frac{1}{(2\pi\hbar)^3} \int d\mathbf{r}_a \int_{t_a}^{t_b} d\tau \int d\mathbf{r} \int d\mathbf{p}_1 \int d\mathbf{p}_2 \times \\ & \times \exp \left\{ -\frac{i\mathbf{p}_1(\mathbf{r}_b - \mathbf{r})}{\hbar} - \frac{ip_1^2(t_b - \tau)}{2m\hbar} \right\} V(|\mathbf{r}|) \exp \left\{ -\frac{i\mathbf{p}_2(\mathbf{r} - \mathbf{r}_a)}{\hbar} - \frac{ip_2^2(\tau - t_a)}{2m\hbar} \right\} \times \\ & \exp \left\{ \frac{i\mathbf{p}_a \mathbf{r}_a}{\hbar} - \frac{iE_a t_a}{\hbar} \right\}. \end{aligned}$$

Further, by integrating over the  $d\mathbf{r}_a, d\tau, d\mathbf{p}_1, d\mathbf{p}_2$  we find

$$\psi_{scat}(\mathbf{r}_b, t_b) = \frac{m}{2\pi\hbar^2} e^{-\frac{iE_b t_b}{\hbar}} \int d\mathbf{r} \frac{\exp \left\{ -\frac{ip_b |\mathbf{r}_b - \mathbf{r}|}{\hbar} \right\}}{|\mathbf{r}_b - \mathbf{r}|} V(|\mathbf{r}|) \exp \left\{ \frac{i\mathbf{p}_a \mathbf{r}}{\hbar} \right\}. \quad (14)$$

When the distance from the origin is much bigger then the effective range for the potential  $V(|\mathbf{r}|)$  it is possible to approximate  $|\mathbf{r}_b - \mathbf{r}| \approx r_b - \mathbf{n}_b \mathbf{r}$  where  $\mathbf{n}_b = \mathbf{r}_b/|\mathbf{r}|$ . Then the Eq.(14) will transformed into the following one

$$\psi_{scat}(\mathbf{r}_b, t_b) = \frac{m}{2\pi\hbar^2} \frac{1}{r_b} \exp\left\{-\frac{iE_b t_b}{\hbar} - \frac{ip_b r_b}{\hbar}\right\} \times \quad (15)$$

$$\int d\mathbf{r} \exp\left\{-\frac{ip_b \mathbf{n}_b \mathbf{r}}{\hbar}\right\} V(|\mathbf{r}|) \exp\left\{\frac{i\mathbf{p}_a \mathbf{r}}{\hbar}\right\}, \quad p_a = p_b.$$

Thus, with the help of Eqs.(10) and (15) the differential cross section defined by Eq.(11) can be read as

$$d\sigma = \left(\frac{m}{2\pi\hbar^2}\right)^2 \left| \int d\mathbf{r} e^{-\frac{i\mathbf{p}_b \mathbf{r}}{\hbar}} V(|\mathbf{r}|) e^{\frac{i\mathbf{p}_a \mathbf{r}}{\hbar}} \right|^2 d\Omega, \quad p_a = p_b \equiv p. \quad (16)$$

This is the well known the first-order Born approximation [16] for the differential scattering cross section.

Introducing the notation  $\mathbf{q}$  for the transferred momentum

$$\mathbf{q} = \mathbf{p}_a - \mathbf{p}_b$$

allows for Eq.(16) to be written as

$$d\sigma = \left(\frac{m}{2\pi\hbar^2}\right)^2 |v(\mathbf{q})|^2 d\Omega, \quad (17)$$

where

$$v(|\mathbf{q}|) = \int d\mathbf{r} V(|\mathbf{r}|) \exp\left\{i\frac{\mathbf{q}\mathbf{r}}{\hbar}\right\},$$

is a Fourier transform of the scattering potential that corresponds to the transferred momentum  $\mathbf{q}$ .

Thus, we have shown how the path integral approach to elastic scattering problem allows to obtain the cross section Eq.(17) in the first-order Born approximation.

### 3 Path integral approach to the electron charge transfer

In this Section we apply the approach developed in the Sec.2 to the electron charge transfer problem.

The classical mechanical action for a system of two heavy particles (resting in the lab system neutral atom A and a moving positive ion B<sup>+</sup>) that exchange an electron between each other can be written as follows

$$S(\mathbf{R}(\tau), \mathbf{r}(\tau)) \quad (18)$$

$$= \int_{t_a}^{t_b} d\tau \left\{ \frac{M \dot{\mathbf{R}}^2(\tau)}{2} + \frac{m \dot{\mathbf{r}}^2(\tau)}{2} - V_A(\mathbf{r}) - V_B(\mathbf{r} - \mathbf{R}) - V_{AB}(\mathbf{R}) \right\}.$$

where  $\mathbf{R}$  is the coordinate of the moving ion B<sup>+</sup>, M is the mass of the ion B<sup>+</sup>,  $\mathbf{r}$  is the coordinate of the electron in the lab frame placed on the resting neutral atom A. In Eq.(18)  $V_A(\mathbf{r})$  is the interaction potential for the system (e<sup>-</sup>+A<sup>+</sup>).  $V_B(\mathbf{r} - \mathbf{R})$  is the interaction potential for the system (e<sup>-</sup>+B<sup>+</sup>) and, at last,  $V_{AB}(\mathbf{R})$  is the interaction potential for the system (B<sup>+</sup>+A<sup>+</sup>).

The transition amplitude  $K(\mathbf{R}_b, \mathbf{r}_b, t_b, \mathbf{R}_a, \mathbf{r}_a, t_a)$  from the "initial" point  $a \equiv (\mathbf{R}_a, \mathbf{r}_a, t_a)$  to the final "point"  $b \equiv (\mathbf{R}_b, \mathbf{r}_b, t_b)$  has the following form

$$K(\mathbf{R}_b, \mathbf{r}_b, t_b, \mathbf{R}_a, \mathbf{r}_a, t_a) = \int D\mathbf{R}(\tau) D\mathbf{r}(\tau) \exp \left\{ \frac{i}{\hbar} S(\mathbf{R}(\tau), \mathbf{r}(\tau)) \right\}. \quad (19)$$

The path integral over two paths  $\mathbf{R}(\tau)$  and  $\mathbf{r}(\tau)$  can be treated by means of the influence functionals. The term influence functional was introduced by Feynman [1]. Indeed suppose we carry out the path integration over the ion trajectories  $\mathbf{R}(\tau)$ . Then the result can be written as

$$K(\mathbf{R}_b, \mathbf{r}_b, t_b, \mathbf{R}_a, \mathbf{r}_a, t_a) = \quad (20)$$

$$\int D\mathbf{r}(\tau) \exp \left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} d\tau \left( \frac{m \dot{\mathbf{r}}^2(\tau)}{2} - V_A(\mathbf{r}(\tau)) \right) \right\} \mathcal{K}_1(\mathbf{R}_b, t_b, \mathbf{R}_a, t_a; \mathbf{r}(\tau)),$$



where the influence functional  $\mathcal{K}_1$  has the form

$$\mathcal{K}_1(\mathbf{R}_b, t_b, \mathbf{R}_a, t_a; \mathbf{r}(\tau)) \quad (21)$$

$$= \int D\mathbf{R}(\tau) \exp \left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} d\tau \left( \frac{M \dot{\mathbf{R}}^2(\tau)}{2} - V_B(\mathbf{r}(\tau) - \mathbf{R}(\tau)) - V_{AB}(\mathbf{R}(\tau)) \right) \right\}.$$

The influence functional  $\mathcal{K}_1(\mathbf{R}_b, t_b, \mathbf{R}_a, t_a; \mathbf{r}(\tau))$  defined by Eq.(21) is in fact transition amplitude for ion under the influence of a potential  $V_B(\mathbf{r}-\mathbf{R})+V_{AB}(\mathbf{R})$  which is computed assuming  $\mathbf{r}(\tau)$  is held to be a fixed path as  $\mathbf{R}(\tau)$  changes. It is obviously that the influence functional  $\mathcal{K}_1(\mathbf{R}_b, t_b, \mathbf{R}_a, t_a; \mathbf{r}(\tau))$  is a functional of  $\mathbf{r}(\tau)$ . Let us represent the influence functional

$\mathcal{K}_1(\mathbf{R}_b, t_b, \mathbf{R}_a, t_a; \mathbf{r}(\tau))$  in the following way

$$\mathcal{K}_1(\mathbf{R}_b, t_b, \mathbf{R}_a, t_a; \mathbf{r}(\tau)) = \exp \left\{ -\frac{i}{\hbar} \int_{t_a}^{t_b} d\tau U_{\mathbf{R}_b, \mathbf{R}_a}(\mathbf{r}(\tau)) \right\}, \quad (22)$$

or

$$\exp \left\{ -\frac{i}{\hbar} \int_{t_a}^{t_b} d\tau U_{\mathbf{R}_b, \mathbf{R}_a}(\mathbf{r}(\tau)) \right\} \quad (23)$$

$$= \int D\mathbf{R}(\tau) \exp \left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} d\tau \left( \frac{M \dot{\mathbf{R}}^2(\tau)}{2} - V_B(\mathbf{r}(\tau) - \mathbf{R}(\tau)) - V_{AB}(\mathbf{R}(\tau)) \right) \right\}.$$

where the effective potential  $U_{\mathbf{R}_b, \mathbf{R}_a}(\mathbf{r})$  has been introduced. Then Eq.(20) can be rewritten as

$$K(\mathbf{R}_b, \mathbf{r}_b, t_b, \mathbf{R}_a, \mathbf{r}_a, t_a) \quad (24)$$

$$= \int D\mathbf{r}(\tau) \exp \left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} d\tau \left( \frac{M \dot{\mathbf{r}}^2(\tau)}{2} - V_A(\mathbf{r}(\tau)) - U_{\mathbf{R}_b, \mathbf{R}_a}(\mathbf{r}(\tau)) \right) \right\}.$$

As a result we have just the path integral over the electron path  $\mathbf{r}(\tau)$ . Thus, Eq.(24) allows treat the electron charge transfer problem as the electron transition under the influence of the perturbation  $V_A(\mathbf{r}) + U_{\mathbf{R}_b, \mathbf{R}_a}(\mathbf{r})$ .

It is possible to introduce another influence functional in the problem of electron charge transfer. Indeed, by integrating over all electron trajectories  $\mathbf{r}(t)$  we find for the transition amplitude  $K(\mathbf{R}_b, \mathbf{r}_b, t_b, \mathbf{R}_a, \mathbf{r}_a, t_a)$  the following equation

$$K(\mathbf{R}_b, \mathbf{r}_b, t_b, \mathbf{R}_a, \mathbf{r}_a, t_a) \quad (25)$$

$$= \int D\mathbf{R}(\tau) \exp \left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} d\tau \left( \frac{M \dot{\mathbf{R}}^2(\tau)}{2} - V_{AB}(\mathbf{R}(\tau)) \right) \right\} \mathcal{K}_2(\mathbf{r}_b, t_b, \mathbf{r}_a, t_a; \mathbf{R}(\tau)),$$

where the influence functional  $\mathcal{K}_2$  is given by

$$\mathcal{K}_2(\mathbf{r}_b, t_b, \mathbf{r}_a, t_a; \mathbf{R}(\tau)) \quad (26)$$

$$= \int D\mathbf{r}(\tau) \exp \left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} d\tau \left( \frac{m \dot{\mathbf{r}}^2(\tau)}{2} - V_A(\mathbf{r}(\tau)) - V_B(\mathbf{r}(\tau) - \mathbf{R}(\tau)) \right) \right\}.$$

The influence functional  $\mathcal{K}_2(\mathbf{r}_b, t_b, \mathbf{r}_a, t_a; \mathbf{R}(\tau))$  defined by Eq.(26) is in fact the electron transition amplitude under the influence of a potential  $V_A(\mathbf{r}) + V_B(\mathbf{r} - \mathbf{R})$  which is computed assuming  $\mathbf{R}(\tau)$  is held to be a fixed path as  $\mathbf{r}(\tau)$  changes. The influence functional  $\mathcal{K}_2(\mathbf{r}_b, t_b, \mathbf{r}_a, t_a; \mathbf{R}(\tau))$  is a functional of ion trajectory  $\mathbf{R}(\tau)$ . It is conveniently to represent the influence functional  $\mathcal{K}_2(\mathbf{r}_b, t_b, \mathbf{r}_a, t_a; \mathbf{R}(\tau))$  in the following way

$$\mathcal{K}_2(\mathbf{r}_b, t_b, \mathbf{r}_a, t_a; \mathbf{R}(\tau)) = \exp \left\{ -\frac{i}{\hbar} \int_{t_a}^{t_b} d\tau V_{\mathbf{r}_b, \mathbf{r}_a}(\mathbf{R}(\tau)) \right\}, \quad (27)$$

or

$$\exp \left\{ -\frac{i}{\hbar} \int_{t_a}^{t_b} d\tau V_{\mathbf{r}_b, \mathbf{r}_a}(\mathbf{R}(\tau)) \right\} \quad (28)$$

$$= \int D\mathbf{r}(\tau) \exp \left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} d\tau \left( \frac{m \dot{\mathbf{r}}^2(\tau)}{2} - V_A(\mathbf{r}(\tau)) - V_B(\mathbf{r}(\tau) - \mathbf{R}(\tau)) \right) \right\}.$$

where the effective potential  $V_{\mathbf{r}_b, \mathbf{r}_a}(\mathbf{R})$  has been introduced.

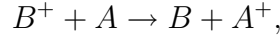
The transition amplitude  $K(\mathbf{R}_b, \mathbf{r}_b, t_b, \mathbf{R}_a, \mathbf{r}_a, t_a)$  can now be written to have only path integration over the ion trajectories  $\mathbf{R}(t)$

$$K(\mathbf{R}_b, \mathbf{r}_b, t_b, \mathbf{R}_a, \mathbf{r}_a, t_a) = \int D\mathbf{R}(\tau) \times \exp \left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} d\tau \left( \frac{M \dot{\mathbf{R}}^2(\tau)}{2} - V_{AB}(\mathbf{R}(\tau)) - V_{\mathbf{r}_b, \mathbf{r}_a}(\mathbf{R}(\tau)) \right) \right\}. \quad (29)$$

This equation allows to consider the charge transfer problem as the elastic scattering of the ion on the effective scattering potential  $V_{AB}(\mathbf{R}) + V_{\mathbf{r}_b, \mathbf{r}_a}(\mathbf{R})$ , where  $V_{\mathbf{r}_b, \mathbf{r}_a}(\mathbf{R})$  is introduced by Eq.(28).

The Eqs.(22)-(24) and (27)-(29) represent the electron charge transfer problem in the terms of the influence functionals  $\mathcal{K}_1(\mathbf{R}_b, t_b, \mathbf{R}_a, t_a; \mathbf{r}(\tau))$  or  $\mathcal{K}_2(\mathbf{r}_b, t_b, \mathbf{r}_a, t_a; \mathbf{R}(\tau))$ .

Let us describe the "rearrangement collision" by means of the path integral approach. Consider the following charge exchange reaction



where  $B^+$  is a projectile and  $A$  is a neutral atom target.

Assuming the center of mass for the system above is at rest, then a classical mechanical action can be written in two alternative ways

$$S_a = \int_{t_a}^{t_b} d\tau (T_a + L_A + L_{B^+} - V_a), \quad (30)$$

$$S_b = \int_{t_a}^{t_b} d\tau (T_b + L_{A^+} + L_B - V_b), \quad (31)$$

where  $L_A, L_{B^+}, L_{A^+}, L_B$  are the Lagrangians of the systems  $A, B^+, A^+, B$ . Here  $T_a$  and  $T_b$  are the kinetic energies of relative motion of systems  $A$  and  $B^+$ , and systems  $A^+$  and  $B$  respectively and, at last,  $V_a$  and  $V_b$  are the perturbations described below.

The geometry of the electron charge transfer problem is shown in Fig. 1. We consider the electron (charge  $-e$  and mass  $m$ ) initially bound to the

heavy particle A of mass  $AM$ , where  $M$  is the mass of a proton. The vector  $\mathbf{R}$  is the position vector of particle  $B^+$  relative to the centre of mass of the electron and the particle A, while  $\mathbf{R}'$  is the position vector of the particle A relative to the centre of mass of the electron and the particle B (see Fig. 1).

As a result of the interaction with the passing ion  $B^+$  of mass  $BM$  the electron is captured into a bound state around the particle B. The action  $S_a$  can be written initially in the form of Eq. (30) with

$$T_a = \frac{\mu_a \dot{\mathbf{R}}^2}{2}, \quad \mu_a = \frac{BM(AM + m)}{(A + B)M + m}, \quad (32)$$

$$L_A = \frac{m_a \dot{\mathbf{r}}^2}{2} - V_A(\mathbf{r}), \quad m_a = \frac{AMm}{AM + m}, \quad (33)$$

where  $V_A(\mathbf{r})$  is the interaction potential between  $A^+$  and  $e^-$ .  $V_a(\mathbf{R}, \mathbf{r})$  describes the interaction between the system  $(A^+ + e^-)$  and  $B^+$ .  $L_{B^+}$  is irrelevant since the ion  $B^+$  is assumed structureless. In the Eq.(30) the coordinates  $\mathbf{r}$  and  $\mathbf{R}$  are in the frame attached to the center of mass of the system  $(A+B^+)$ .

The action  $S_b$  can be rearranged for the final configuration into the form of Eq.(31) with

$$T_b = \frac{\mu_b \dot{\mathbf{R}}'^2}{2}, \quad \mu_b = \frac{AM(BM + m)}{(A + B)M + m}, \quad (34)$$

$$L_B = \frac{m_b \dot{\mathbf{r}}'^2}{2} - V_B(\mathbf{r}'), \quad m_b = \frac{BMm}{BM + m}, \quad (35)$$

where  $V_B(\mathbf{r}')$  is the interaction potential between  $B^+$  and  $e^-$ .  $V_b(\mathbf{R}', \mathbf{r}')$  describes the interaction between  $A^+$  and the system  $(B^+ + e^-)$ .  $L_{A^+}$  is irrelevant since the ion  $A^+$  is assumed structureless. Again, in the Eq.(31) the coordinates  $\mathbf{r}'$  and  $\mathbf{R}'$  are in the frame attached to the center of mass of the system  $(A^+ + B)$ .

Once the action is known it is possible to construct the transition amplitude  $K(b, a)$  that describes the relative motion of the neutral atom, ion and the transition of the electron from the neutral atom to the positive ion,

$$K_a(\mathbf{R}_b, \mathbf{r}_b, t_b, \mathbf{R}_a, \mathbf{r}_a, t_a) \quad (36)$$

$$= \int D\mathbf{R}(\tau) D\mathbf{r}(\tau) \exp \left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} d\tau (T_a + L_A + L_{B^+} - V_a) \right\},$$

or

$$K_b(\mathbf{R}'_b, \mathbf{r}'_b, t_b, \mathbf{R}'_a, \mathbf{r}'_a, t_a) \quad (37)$$

$$= \int D\mathbf{R}'(\tau) D\mathbf{r}'(\tau) \exp \left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} d\tau (T_b + L_{A^+} + L_B - V_b) \right\}.$$

Further it is possible to represent the wave function  $\Phi(\mathbf{R}_a, \mathbf{r}_a, t_a)$  of the interacting (rearrangement collision) particles as follows

$$\Phi(\mathbf{R}_a, \mathbf{r}_a, t_a) = \varphi_{n_a}(\mathbf{r}_a) \Psi(\mathbf{R}_a, t_a), \quad (38)$$

$$\Psi(\mathbf{R}_a, t_a) = \exp \left\{ \frac{i \mathbf{p}_a \mathbf{R}_a}{\hbar} - \frac{i E_a t_a}{\hbar} \right\}, \quad (39)$$

here  $\varphi_{n_a}$  is the wave function of the electron bound to the nucleus A,  $\Psi(\mathbf{R}_a, t_a)$  is the wave function of the relative motion ( $A^+ + e^-$ ) and  $B^+$ ,  $\mathbf{p}_a$  and  $E_a$  are the momentum and the energy respectively of the relative motion ( $A^+ + e^-$ ) and  $B^+$ . The total energy of the system that enters the reaction is

$$E_a^{tot} = E_a + \varepsilon_a,$$

here  $\varepsilon_a$  is the energy of the electron bound to the nucleus  $A^+$ . As a result of the rearrangement collision the system in the outgoing canal consists of the  $A^+$  and the electron bound to the ion  $B^+ + e^-$ . In this final state the total energy of the system is

$$E_b^{tot} = E_b + \varepsilon_b,$$

where  $E_b$  is the energy of the relative motion of the  $A^+$  and ( $B^+ + e^-$ ) after the charge transfer reaction and  $\varepsilon_b$  is the binding energy of the electron to the ion  $B^+$ . Due to the energy conservation

$$E_a^{tot} = E_b^{tot}$$

it follows that the energy of the relative motion after the charge transfer reaction is

$$E_b = E_a + \varepsilon_a - \varepsilon_b.$$

Different final states of the system (states with different quantum numbers) are called the reaction channels. The channel is called "open channel" if the following condition is satisfied.

$$E_a + \varepsilon_a - \varepsilon_b \geq 0.$$

In this case the energy of the relative motion of the particles after the reaction is positive and hence they can fly apart to infinity. If there is the opposite sign in the above equation

$$E_a + \varepsilon_a - \varepsilon_b \leq 0,$$

then the channel is called "closed channel".

The evolution of the quantum mechanical system is defined by the wave function  $\Phi(\mathbf{R}_b, \mathbf{r}_b, t_b)$ . The transition amplitude (36) or (37) and the initial state of the system (wave function (38)) will fully define the  $\Phi(\mathbf{R}_b, \mathbf{r}_b, t_b)$  for the system ( $A^+ + e^-$ ) and  $B^+$

$$\Phi(\mathbf{R}_b, \mathbf{r}_b, t_b) = \int d\mathbf{R}_a d\mathbf{r}_a K_b(\mathbf{R}_b, \mathbf{r}_b, t_b, \mathbf{R}_a, \mathbf{r}_a, t_a) \Phi(\mathbf{R}_a, \mathbf{r}_a, t_a), \quad (40)$$

where the transition amplitude  $K_b(\mathbf{R}_b, \mathbf{r}_b, t_b, \mathbf{R}_a, \mathbf{r}_a, t_a) \equiv K(b, a)$  is defined according to (37).

In order to specify the charge transfer process it is necessary to transform the wave function (40) in such a way that it behaves as the scattered spherical wave in the limit  $R_b \rightarrow \infty$ . Taking into consideration Eq.(40) we can define the new wave function  $\Phi_{ch-tr}(\mathbf{R}_b, \mathbf{r}_b, t_b)$  as follows

$$\Phi_{ch-tr}(\mathbf{R}_b, \mathbf{r}_b, t_b) = \int d\mathbf{R}_a d\mathbf{r}_a \{K(b, a) - K^{(0)}(b, a)\} \Phi(\mathbf{R}_a, \mathbf{r}_a, t_a), \quad (41)$$

where the transition amplitude  $K^{(0)}(b, a)$  is given by

$$\begin{aligned} K^{(0)}(b, a) &= \int D\mathbf{R}(\tau) D\mathbf{r}(\tau) \exp \left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} d\tau (T_a + L_A + L_{B^+}) \right\} = \\ &= \int D\mathbf{R}'(\tau) D\mathbf{r}'(\tau) \exp \left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} d\tau (T_b + L_{A^+} + L_B) \right\}. \end{aligned} \quad (42)$$

The charge transfer cross section can be defined as the ratio of the flux of ions (that went through the charge change process and scattered into the solid angle  $d\Omega$  per unit time) to the initial flux of the ions. There are  $j_b R_b^2 d\Omega$  ions (went through the charge exchange process region) go through the area  $R_b^2 d\Omega$  per unit time. Here  $j_b$  is the radial component of the flux defined as follows

$$j_b = \frac{\hbar}{2\mu_b i} \left( \Phi_{ch-tr}^* \frac{\partial}{\partial R_b} \Phi_{ch-tr} - \Phi_{ch-tr} \frac{\partial}{\partial R_b} \Phi_{ch-tr}^* \right), \quad (43)$$

where  $\Phi_{ch-tr}$  is given by the Eq.(41) and  $\mu_b$  is defined in according to Eq.(34). The initial ion flux is equal to the velocity of the ions due to the normalization of the wave function Eq.(39)

$$\mathbf{j}_a = \frac{\mathbf{p}_a}{\mu_a}. \quad (44)$$

Hence we have come to the following definition for the charge transfer differential cross section

$$d\sigma = \frac{j_b R_b^2 d\Omega}{|\mathbf{j}_a|}, \quad (45)$$

where  $\mu_a$  is given by Eq.(32).

The Eqs.(38), (41), (43)-(45) represent the formulation of the charge transfer process in terms of the Feynman path integral.

Let us show that the developed approach used in the first order of the perturbation theory will lead to the well known charge transfer cross section formula [12], [17].

If the Eq.(41) is expanded in series of the potential only to the first order then the transition amplitude  $K_a(b, a)$  can be written as below

$$K(b, a) = \int D\mathbf{R}(\tau) D\mathbf{r}(\tau) \exp \left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} d\tau (T_b + L_A + L_{B^+}) \right\} \times \quad (46)$$

$$\left( 1 - \frac{i}{\hbar} \int_{t_a}^{t_b} d\tau V_a(\mathbf{R}(\tau), \mathbf{r}(\tau)) \right),$$

or as

$$K(b, a) = \int D\mathbf{R}'(\tau) D\mathbf{r}'(\tau) \exp \left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} d\tau (T_b + L_{A^+} + L_B) \right\} \times \quad (47)$$

$$\left( 1 - \frac{i}{\hbar} \int_{t_a}^{t_b} d\tau V_b(\mathbf{R}'(\tau), \mathbf{r}'(\tau)) \right).$$

Then

$$\Phi_{ch-tr}(\mathbf{R}_b, \mathbf{r}_b, t_b) = -\frac{i}{\hbar} \int d\mathbf{R}_a d\mathbf{r}_a \int_{t_a}^{t_b} d\tau \int d\mathbf{R} d\mathbf{r} K^{(0)}(\mathbf{R}_b, \mathbf{r}_b, t_b, \mathbf{R}, \mathbf{r}, \tau) \times \quad (48)$$

$$V_{(a,b)}(\mathbf{R}, \mathbf{r}) K^{(0)}(\mathbf{R}, \mathbf{r}, \tau, \mathbf{R}_a, \mathbf{r}_a, t_a) \varphi_{n_a}(\mathbf{r}_a) \Phi(\mathbf{R}_a, t_a),$$

where  $K^{(0)}$  is defined by Eq.(42).

Further, following almost exactly the same procedure that led from Eq.(13) to Eq.(16) we write  $\Phi_{ch-tr}$  in the form

$$\Phi_{ch-tr}(\mathbf{R}_b, \mathbf{r}_b, t_b) = \frac{\mu_b}{2\pi\hbar^2} \exp \left\{ -i \frac{(E_b + \varepsilon_a - \varepsilon_b)t_b}{\hbar} - i \frac{\mathbf{p}_b \mathbf{R}_b}{\hbar} \right\} \times \quad (49)$$

$$\int d\mathbf{R} d\mathbf{r} e^{-i \frac{\mathbf{p}_b \mathbf{R}}{\hbar}} \phi_{n_b}^*(\mathbf{r}) \times V_{(a,b)}(\mathbf{R}, \mathbf{r}) e^{i \frac{\mathbf{p} \mathbf{R}}{\hbar}} \phi_{n_a}(\mathbf{r}),$$



where  $\varphi_{n_a}(\mathbf{r})$  is the wave function of the electron bound to nucleus A and  $\varphi_{n_b}(\mathbf{r})$  is the wave function of the electron bound to the nucleus B, and  $\mu_b$  is given in according to Eq.(34). Substituting the Eq.(49) for  $\Phi_{ch-tr}(\mathbf{R}_b, \mathbf{r}_b, t_b)$  in the definition (43) and taking into account Eqs.(44) and (45) we have the following equation

$$d\sigma = \left(\frac{\mu_b}{2\pi\hbar^2}\right)^2 \cdot \left(\frac{p_b}{p_a}\right)^2 \left| \int d\mathbf{R} d\mathbf{r} e^{-i\frac{\mathbf{p}_b \mathbf{R}}{\hbar}} \phi_{n_b}^*(\mathbf{r}) V_{(a,b)}(\mathbf{R}, \mathbf{r}) e^{i\frac{\mathbf{p}_a \mathbf{R}}{\hbar}} \phi_{n_a}(\mathbf{r}) \right|^2 d\Omega. \quad (50)$$

where  $p_a$  and  $p_b$  are the absolute values of the initial and the final momentums of moving ion.

Thus we obtain the differential cross section for the electron charge transfer process in the first-order Born approximation [12], [13], [17], [18]. Hence we have shown that the path integral approach allows to obtain the well-known results for the electron charge transfer problem.

## 4 Conclusions

The path integrals approach is applied to atomic physics problem. The electron charge transfer has been studied by means of the path integral approach. We have developed the influence functional treatment of the electron charge transfer process either as an electron transition problem or as an elastic scattering of ion and atom in the some effective potential. It has been shown how the first Born approximation for the elastic scattering cross section can be derived by path integral approach. For the charge transfer reaction the differential cross section in the first Born approximation has been obtained to prove the adequacy of the path integrals approach to this problem.

## 5 Acknowledgments

We would like to thank the IsoTrace Lab. and especially to Prof. Ted Litherland for his interest in the development of new ideas, numerous stimulating discussions and the financial support of this work.

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